HFBTHO installation instructions

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HFBTHO is an axial code for solving the Hartree-Fock-Bogoliubov equations in a harmonic-oscillator basis. For this exercise, we will be using the version 3.0 of the code. Although not the most recent version, it has all the required physics and it compiles straightforwardly on Ubuntu and lxplus (v4 has raised some issues).

The **source files** required to compile the program are available here, HFBTHO3.zip, together with the manual of the code. The HFBTHO code is open source and can be found online, but it is better to use the provided version, which has a few modifications in the way the code is executed and the resulting output files (see at the end).

Compilation prerequisites:

To compile the code, one requires a Linux distribution. Recently the code was successfully compiled on Ubuntu Desktop 24. Probably any maintained Ubuntu distribution should work. The code was also successfully compiled on the server lxplus.cern.ch (which can be an option for participants with an lxplus account).

On Windows, the simplest solution is to emulate Ubuntu with a Virtual Machine (for example VirtualBox or VMWare, both free). For running simple calculations with the code, a virtual machine with 2 CPUs and 4 GB RAM memory is enough, but double is better if possible.

Once logged into Ubuntu, a number of packages are necessary for the compilation and if not present they can be installed in a terminal with:

sudo apt-get install [package_name]

The package names are:

- python3 (*should be by default present on Ubuntu*)
- gfortran
- liblapack-dev
- libblas-dev
- meson (*perhaps not needed*)
- pkg-config (*perhaps not needed*)
- doxygen

Verify where the "liblapack.a" and "libblas.a" are located on your system:

dpkg -L liblapack-dev

dpkg -L libblas-dev

In the "home" folder, create the folder "local". Navigate to the folder in the terminal and inside create the following symbolic links:

ln -s [path_to_blas_folder]/libblas.a libblas.a

ln -s [path_to_lapack_folder]/liblapack.a liblapack.a

For the Ubuntu 24 example, the two libraries are by default placed in the folders.

/usr/lib/x86_64-linux-gnu/blas

/usr/lib/x86_64-linux-gnu/lapack

which means the links to make are:

ln -s /usr/lib/x86_64-linux-gnu/blas/libblas.a libblas.a

ln -s /usr/lib/x86_64-linux-gnu/lapack/liblapack.a liblapack.a

Compiling the code

Extract the HFBTHO3.zip archive in the "home" folder (or any subfolder of it). Navigate in a terminal to the "source" subfolder and type

make

Normally the Makefile is already correctly configured for the required usage of the code.

Running the code

After successful compilation, to run the code one needs to use

./hfbtho_main [input_file]

Please note that this is different from what the Readme file specifies. This is because the code was slightly modified from its original version, to make it compatible with cluster runs. An input file is already prepared in the source folder, called hfbtho_NAMELIST.dat. To check that the code runs properly with a quick calculation, one can thus run:

./hfbtho_main hfbtho_NAMELIST.dat

The calculation will run and the detailed code output will be written in the file

hfbtho_NAMELIST.dat.out

while a summary of the main results of interest will be written to

hfbtho_NAMELIST.dat.sum

Questions and troubleshooting

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